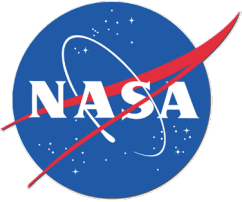


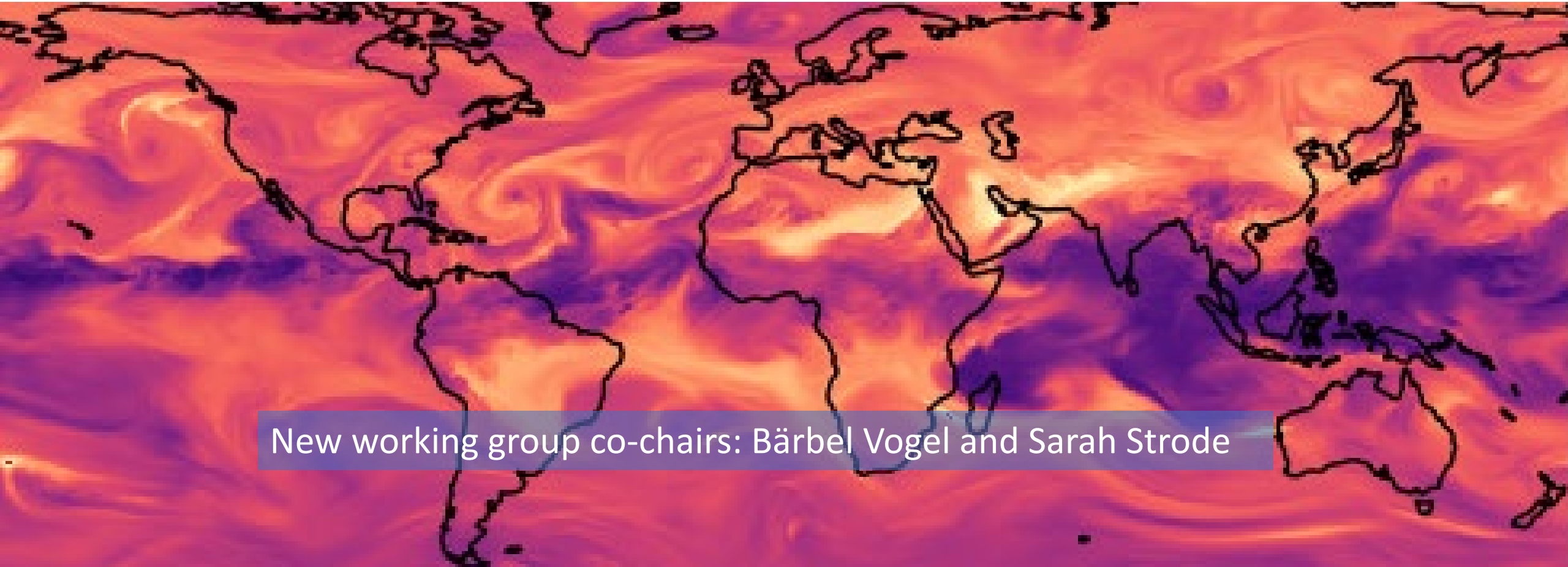
Theory and Analysis Working Group



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²Karlsruhe Institute of Technology

A world map with a color-coded overlay representing atmospheric data, likely temperature or pressure, showing swirling patterns across the continents and oceans. The colors range from dark purple to bright orange.

New working group co-chairs: Bärbel Vogel and Sarah Strode

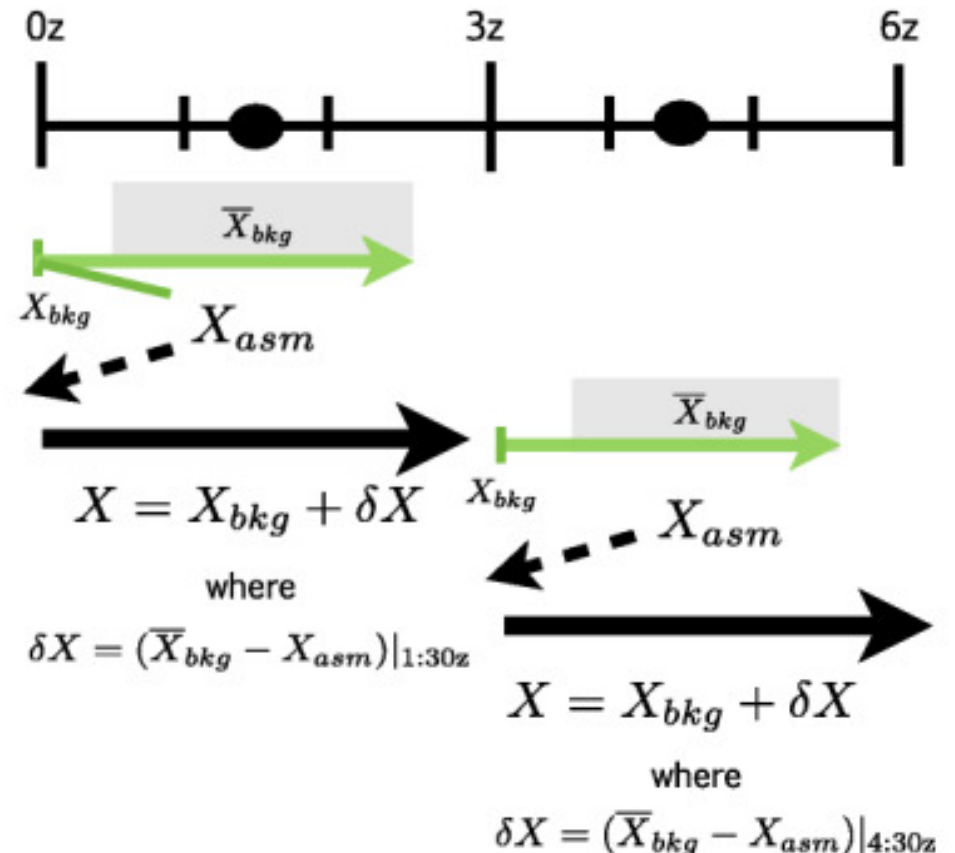
Status of Model Output for NDACC

- Output from the Global Modeling Initiative (GMI) is provided to support NDACC analyses
 - Many thanks to Susan Strahan for her effort over the years!
- GMI chemistry mechanism includes over 120 species, ~400 reactions
- GMI runs within chemistry and transport model (CTM) and chemistry climate model (CCM) frameworks
- Most recent update: Spring 2023
 - Higher resolution CCM replay simulation: c360 (~25km)
- Vertical profiles extracted at NDACC stations :
 - 3-hourly O₃, NO₂, water, temperature, pressure, potential vorticity, tropopause pressure, and age of air interpolated to geometric altitude
 - 24-hour averages of FTIR species on pressure levels

CTM to Replay transition

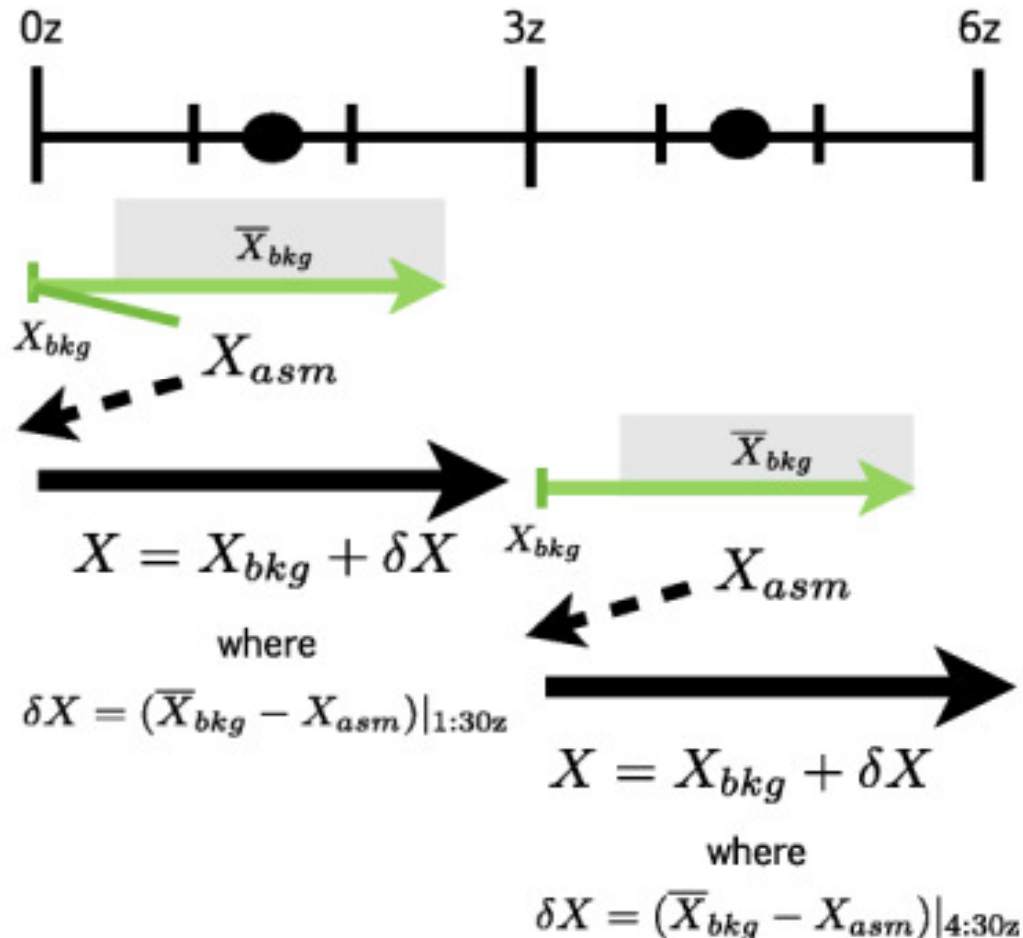
- Traditionally, GMI NDACC output came from CTM simulations, where reanalysis meteorological fields were read in
- Latest submission comes from a “Replay” simulation of the GEOSCCM: CCM simulation with meteorology constrained by (replayed to) reanalysis fields

Replay Method



Orbe et al (2017)

Replay Method



Model runs forward to make a prediction (green arrow)

average over gray window gives $\bar{X}_{bkg}$

Compare to assimilated state: $\delta X = (\bar{X}_{bkg} - X_{asm})|_{1:30z}$

Rewind back to 0z

Run forward again for 3 hours, adding in δX to create new X_{bkg} for 3z

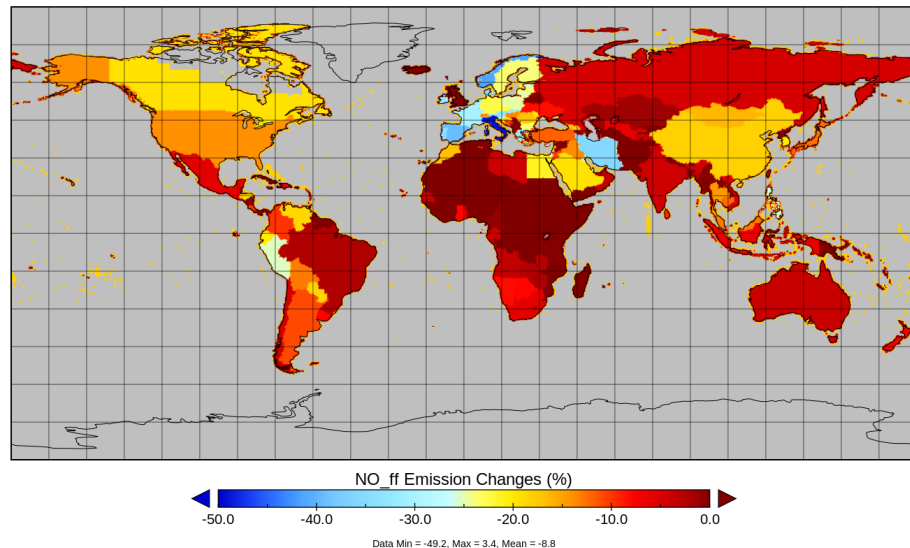
Repeat for the next 3 hour segment

Intended to be functionally similar to a CTM

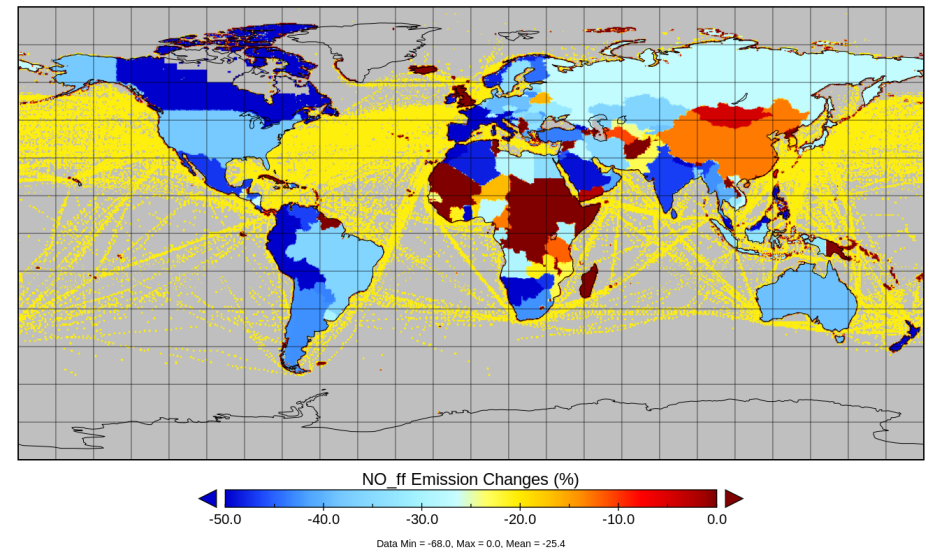
Replay simulation

- “MINDS” GEOSCCM simulation (courtesy of Luke Oman) with GMI chemistry and GOCART aerosols replayed to MERRA2 meteorology
- Available 1996-2022, additional years may be available in the future
- Emissions change over time, include COVID-related updates

Mid-March 2020 Emission Changes (2020-2019)

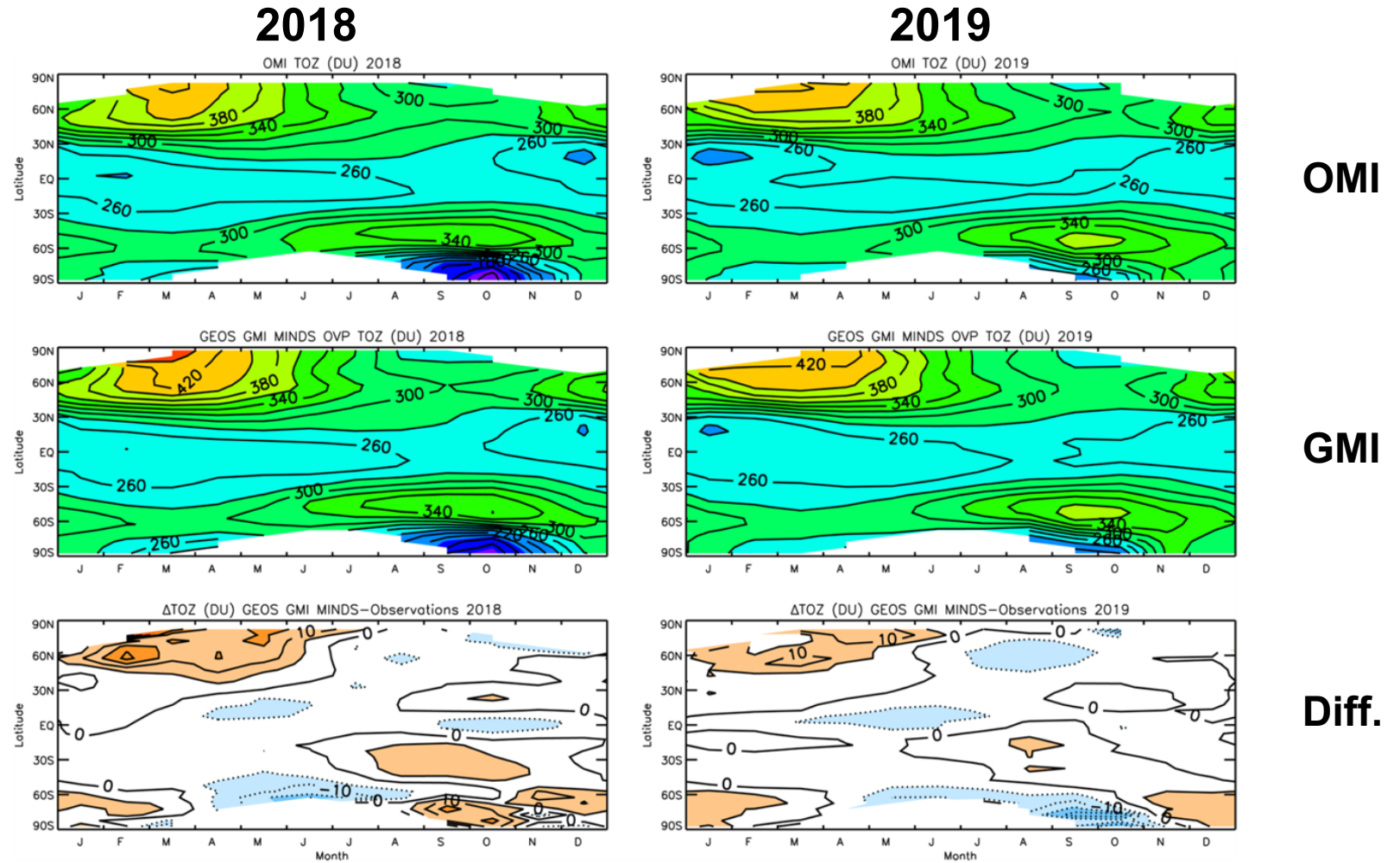


Mid-April 2020 Emission Changes (2020-2019)



GEOS GMI Provides Well Simulated Total Column Ozone Across the Seasonal Cycle

- The simulation difference with OMI total column ozone over the seasonal cycle is typically less than ± 5 DU (~1-2%) **outside of the polar regions** in winter and spring
- In the Antarctic spring these examples are from a strong ozone loss year (2018) and a weak ozone loss year (2019)
- A tropospheric ozone high bias explains part of the high Arctic O_3 in NH winter and spring (recently addressed)

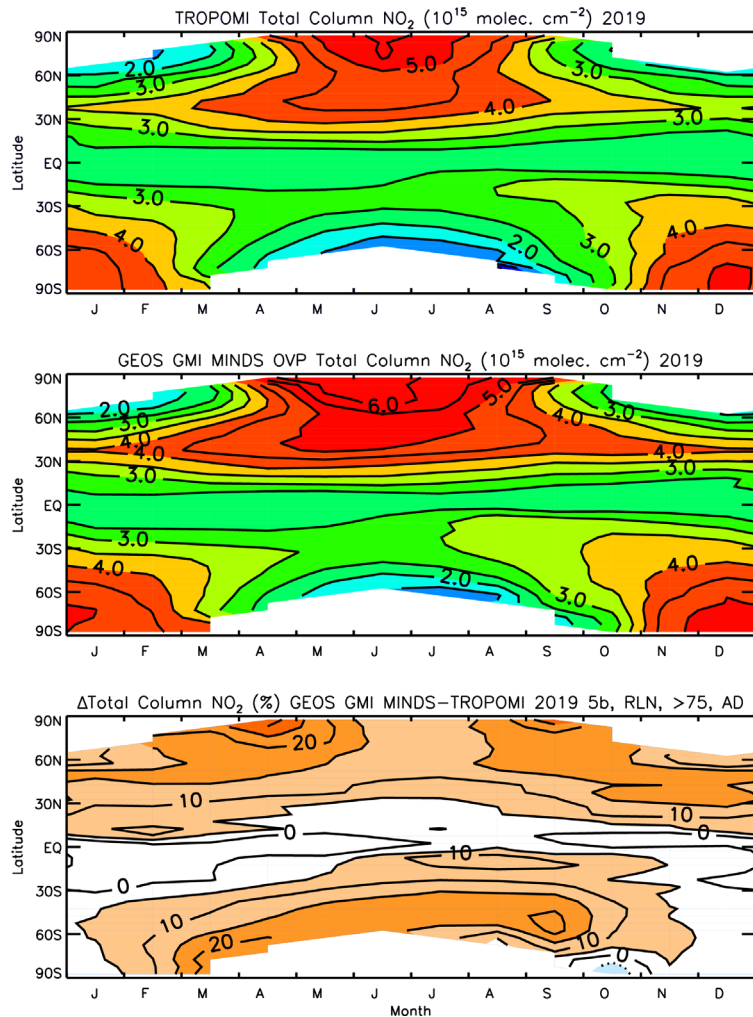


The figure above shows the total column ozone (DU) from OMI (top) compared to the simulated GEOS GMI (middle) and difference (bottom) for 2018 (left) and 2019 (right).

c.o. L. Oman

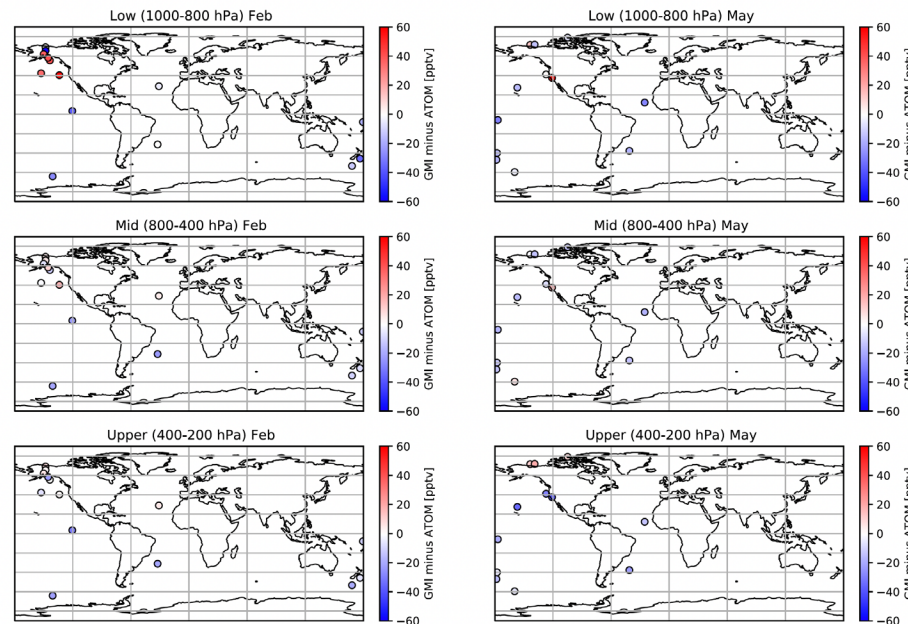
Model NO₂ Evaluations Against Orbital, Sub-orbital, and Ground-based Measurements

TROPOMI Measurements

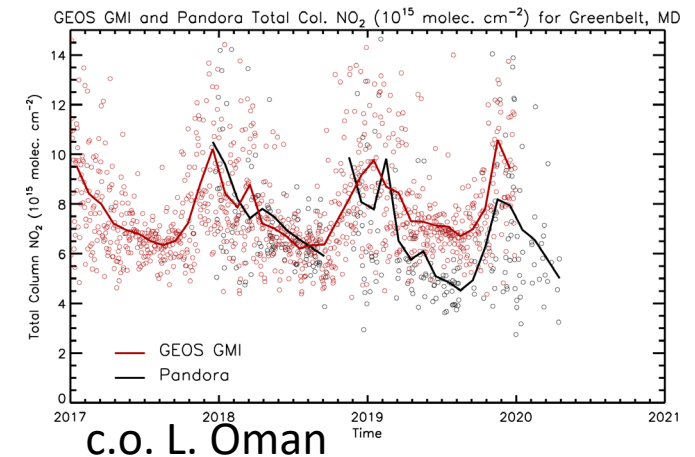
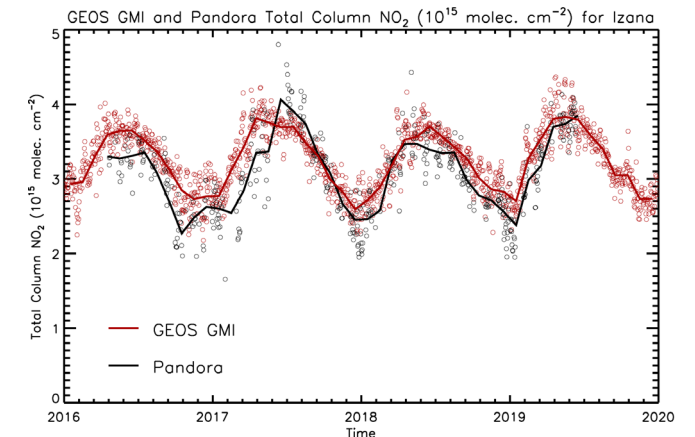


We generally see a small high bias in total column measurements and a low bias in remote tropospheric locations

ATom Profile Measurements



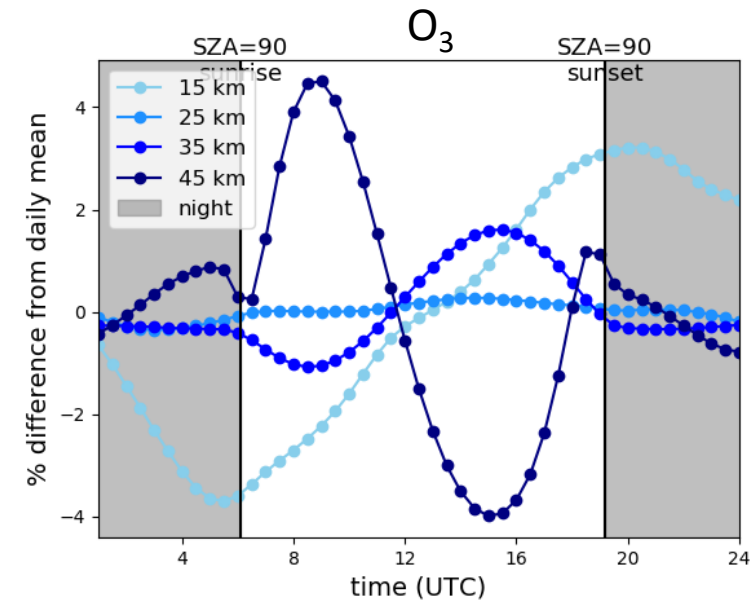
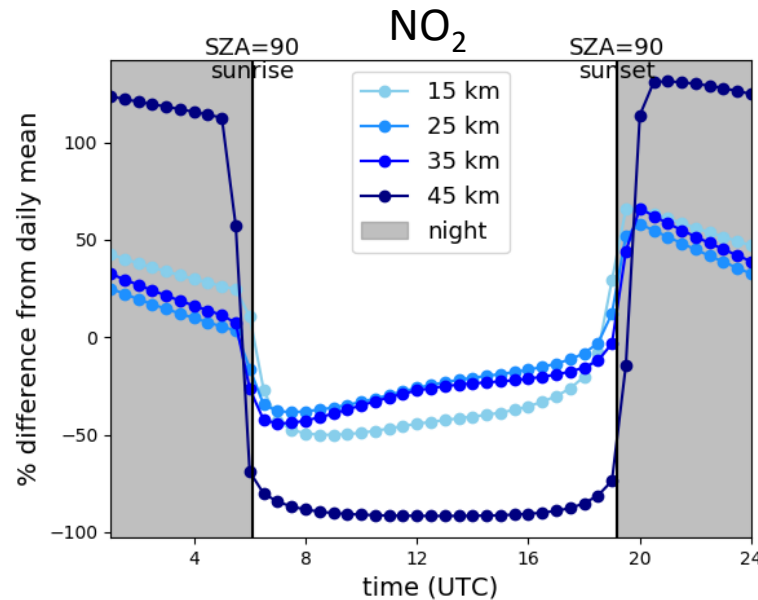
Pandora Site Measurements



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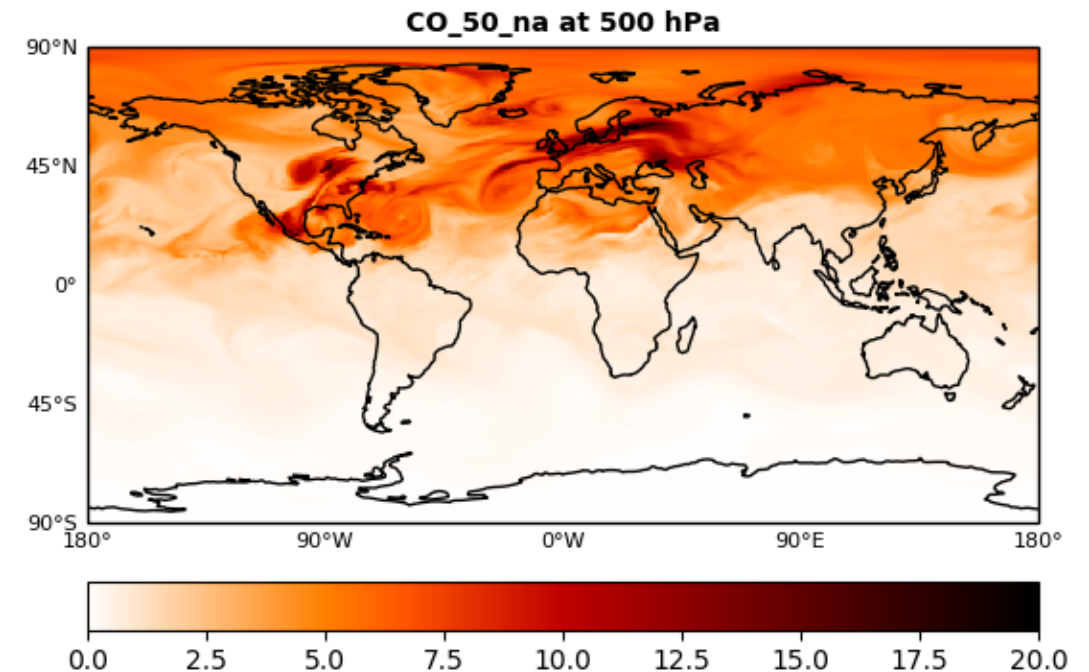
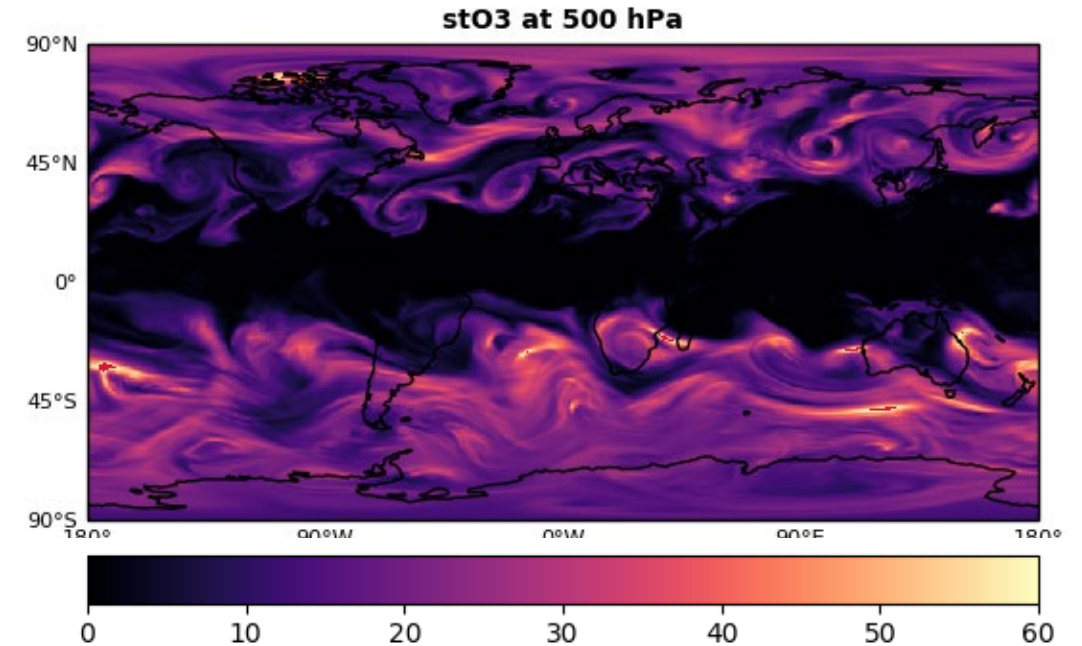
Simulations provide global and temporal context

- Trends across different observing periods
- Representativeness of specific locations
- Simulated diurnal cycle for intercomparing observations at different times of day
 - For example, Strode et al (2022) created diurnal scaling factors for O_3 and NO_2 as a function of SZA and altitude



Idealized tracers

- In addition to chemical species & aerosols, the simulation includes tracers that represent particular processes or transport from specific regions
- stratO3: tracer of stratospheric ozone influence in the troposphere; loss (but not production) applied in the troposphere
- CO_50_na, CO_50_ea, etc.: CO-like tracers with a 50-day lifetime emitted from a specific region to identify regional contributions
- Other examples: age of air, CH₃I (for marine convection), st80_25, nh_5



Links to CCMI and Intercomparisons

- Observations provide a valuable source of validation for model intercomparison projects
- The chemistry climate model intercomparison project (CCMI) includes both “specified dynamics” simulation, which use specified meteorology (via CTM, “replay”, or nudging) and free-running simulation where models simulate the meteorology
- Specified dynamics case allows matching specific dates/meteorology; free-running CCMs require more statistical comparisons

Action Items and Discussion

- Website ndacc-theory.org, still hosted by Björn-Martin, needs to be updated and relocated
- Propose to have 1-2 virtual meetings per year to broaden the Theory and Analysis Work group
 - Theory & Analysis co-chairs and alumni
 - representative for operational data use
 - invited expert for greenhouse gas modelling
 - Invited expert from CMIP or CCMI
 - additional invited experts as needed

Discussion topic: Would additional output be useful?

- Would the full global fields (not extracted to specific NDACC sites) be useful?
- Large data volume, but subsets could be available on request
- Provides spatial and temporal context
- Are additional species also useful? Aerosols or idealized tracers?

Discussion topic: Simulation time periods and Acknowledgement

- How important is it to have up-to-date simulations (simulate most recent years with current model version) versus consistent long-term simulations (multi-decade simulation with a single model version)?
 - The former can be done more frequently, but has potential for discontinuities between earlier and later years
 - The latter is done less frequently, but yields a self-consistent time series
- Please keep us in the loop if you are using NDACC model outputs in your work
 - helpful to show our program managers how products they fund are used in the international community
 - We can keep abreast of the observations and interact about model issues